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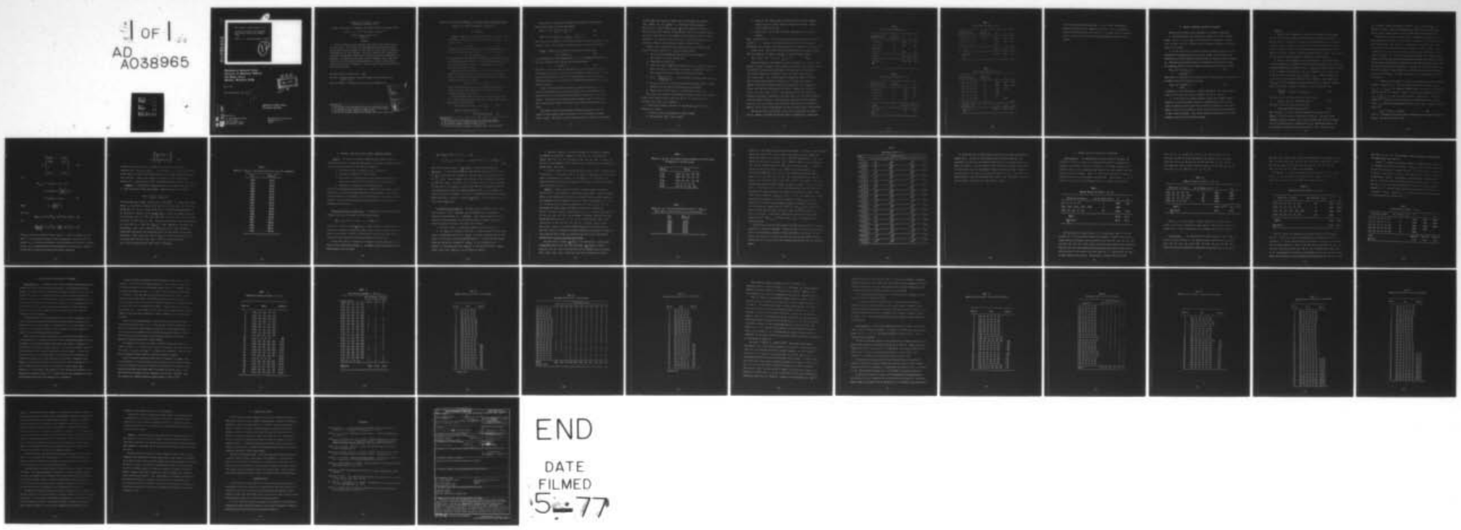

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Ralph C. St. John and Norman R. Draper

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Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53706

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DESIGNS IN FIVE AND SIX COMPONENTS FOR MIXTURES MODELS WITH INVERSE TERMS*

Ralph C. St. John[3,4] and Norman R. Draper[1,2,3]

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ABSTRACT

Briefly reviewed are the polynomial plus inverse terms mixture models of Draper and St. John (1977a), and the approximately D-optimal (measure) and D_n-optimal (exact) designs for these models in three and four components (see Draper and St. John (1977b)). The use of Atwood's (1973) improvement to Fedorov's D-optimality algorithm is reviewed and further improvements are suggested. In addition, design region and model symmetry, and a simplified procedure for re-distributing design measure, are used to obtain measure designs in five and six components. Finally, exact designs are obtained from these measure designs.

AMS (MOS) Subject Classification: 62K05

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DESIGNS IN FIVE AND SIX COMPONENTS FOR MIXTURES MODELS WITH INVERSE TERMS

Ralph C. St. John[3,4] and Norman R. Draper[1,2,3]

1. BACKGROUND

Mixtures. Suppose η is a response which depends on $\underline{x}$, a set of q predictor or independent variables, and $\underline{\theta}$, a set of unknown parameters, through an unknown response function.

$$\eta = g(\underline{x},\underline{\theta}). \qquad (1)$$

In observing the response η we assume that additive experimental error, denoted by ε, exists so that, for each observation y_i, $i = 1,2\ldots n$, we can write

$$y_i = \eta_i+\varepsilon_i = g(\underline{x}_i,\underline{\theta}) + \varepsilon_i. \qquad (2)$$

We assume that the ε_i are independently and identically distributed with means zero and variance-covariance matrix $\sigma^2\underline{I}$. In many cases where the form of the true response function (1) is unknown, it is approximated by a polynomial function of as low order as possible.

Suppose that the response depends only on the relative proportions of the independent variables x_i, and not on the total amount of each independent variable. Then without loss of generality we may suppose that the predictor variables are restricted to the region

$$\chi = \{\underline{x} \mid x_i > 0,\ i=1,2\ldots q;\ \sum_{i=1}^{q} x_i = 1\}, \qquad (3)$$

In this case we have a mixture problem, and the x_i's are called components of the mixture. Cornell (1973) and Draper and St. John (1974) review the literature of experiments with mixtures.

The usual polynomial models are not directly applicable to mixture problems. Scheffé (1958, 1963) suggested these first and second order canonical polynomials for use with mixtures:

Linear canonical polynomial $\quad E(y) = \sum_{i=1}^{q} \beta_i x_i \qquad (4)$

Quadratic canonial polynomial

$$E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j}\sum \beta_{ij} x_i x_j \qquad (5)$$

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Draper and St. John (1977a) extended these canonical polynomials by adding inverse terms to obtain these models:

$$\text{MODEL I} \quad E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{-i} x_i^{-1} \tag{6}$$

$$\text{MODEL II} \quad E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j} \beta_{ij} x_i x_j + \sum_{i=1}^{q} \beta_{-i} x_i^{-1} \tag{7}$$

These models are intended for use in mixture problems where the response changes rapidly as some of the components approach but do not reach given boundaries.

Design. Suppose one is willing to entertain the linear model

$$y_i = \underline{f}'(\underline{x}_i)\underline{\beta} + \varepsilon_i \tag{8}$$

as an approximation of the unknown model (2). If n experimental observations are to be obtained, we can express this in matrix form as

$$\underline{y} = \underline{X\beta} + \underline{\varepsilon}. \tag{9}$$

The vector y is an nx1 vector of observations; X is an nxp matrix, with row i containing $\underline{f}'(\underline{x}_i)$; $\underline{x}_i$ is a qx1 vector of independent variables; $\underline{f}(\underline{x}_i)$ is a px1 vector which specifies the form of the assumed model; $\underline{\beta}$ is a px1 vector of unknown parameters; $\underline{\varepsilon}$ is an nx1 vector of random errors (assumptions on the ε_i's were given above).

Given n the design problem consists of selecting vectors $\underline{x}_i$, 1,2...n, from the appropriate design region (for example, (3) for standard mixtures problems) such that the design defined by these n vectors is, in some sense, optimal. One criterion for obtaining such a design is that of D-optimality, which simply stated, leads to selection of the n vectors which maximize det $(\underline{X}'\underline{X})$.

The design concept was generalized by Kiefer and Wolfowitz (1959) to allow for specifiying a design as a measure ξ over the appropriate design region, say $\mathcal{X}$. The measure ξ places positive measure at points to be included

in the design, zero measure at points not in the design, and satisfies $\xi(\underline{x}) \geq 0, \forall\ \underline{x} \in \mathcal{X}$, and $\int_{\mathcal{X}} \xi(d\underline{x}) = 1$. The measure design analog of $\underline{X}'\underline{X}$ is $\underline{M}(\xi_1) = [m_{ij}(\xi)]$ where $m_{ij}(\xi) = \int_{\mathcal{X}} f_i(\underline{x}) f_j(\underline{x}) \xi(d\underline{x})$ for all i,j. Measure designs which maximize the determinant of $\underline{M}(\xi)$ are called D-optimal, and exact n-point designs, which maximize the determinant of $\underline{X}'\underline{X}$ are called D_n-optimal. St. John and Draper (1975) give a review of D-optimality for regression problems, and as applied to mixture problems (1974).

Briefly, the construction of D-optimal measure designs follows these steps (see Fedorov (1972) or St. John and Draper (1975)):

1. Let ξ_n be any nondegenerate ($\det \underline{M}(\xi_n) > 0$) n-point design on $\mathcal{X}$, and let i=n in the initial step.
2. Compute $\underline{M}(\xi_i)$ and $\underline{M}^{-1}(\xi_i)$.
3. Select the point from $\mathcal{X}$ which maximizes $d(\underline{x}, \xi_i) = \underline{f}'(\underline{x})\, \underline{M}^{-1}(\xi_i)\, \underline{f}(\underline{x})$, (Note that $d(\underline{x}, \xi_i)$ is analogous to $V(\hat{y}(\underline{x})) = \underline{f}'(\underline{x})(\underline{X}'\underline{X})^{-1}\underline{f}(\underline{x})$.) and let $\underline{x}_i$ be the point at which this maximum is attained.
4. Let $\alpha_i = \dfrac{d(\underline{x}_i, \xi_i) - p}{p\,(d(\underline{x}_i, \xi_i) - 1)}$ be the measure at the new design point $\underline{x}_i$.
5. Let $\xi_{i+1} = (1-\alpha_i)\,\xi_i + \alpha_i \delta$ be the new design measure (where δ places measure one at the point $\underline{x}_i$ and measure zero elsewhere.)
6. Repeat steps 2-5 until $d(\underline{x}_i, \xi_i)$ is sufficiently close to p.

This algorithm is based on the equivalence theorem of Kiefer and Wolfowitz (1959), which states (in part) that $\max d(\underline{x}, \xi) = p$ if and only if ξ is D-optimal and $\max d(\underline{x}, \xi) > p$ otherwise.

A single-point exchange procedure for constructing D_n-optimal exact designs is as follows:

1. **Select an arbitrary nondegenerate n-point design.**
2. **Calculate $\underline{X}'\underline{X}$, $(\underline{X}'\underline{X})^{-1}$ and $\det(\underline{X}'\underline{X})$.**

3. Select $\underline{x}^* \in \mathcal{X}$ and $\underline{x}_k$ from the current design such that exchange of $\underline{x}^*$ for $\underline{x}_k$ will give the largest increase in det $(\underline{X}'\underline{X})$. Add $\underline{x}^*$ to the design and drop $\underline{x}_k$.

4. Repeat steps 2 and 3 until no further improvement in det $(\underline{X}'\underline{X})$ is possible.

Note: We have "omitted" σ^2 in the variance expressions given above, that is, assumed $\sigma^2 = 1$. Because we are only interested in the relative values of determinants and variances, the optimal designs do not depend on the value of σ^2.

Draper and St. John (1977b) have given measure and exact designs in three and four components for Model I and Model II when the design region is

$$\mathcal{X}_1 = \{\underline{x} | x_i \geq .05,\ i = 1,2\ldots q;\ \sum_{i=1}^{q} x_i = 1\}. \qquad (10)$$

Measure designs for these models are given in Tables 1, 2, 3, and 4. The designs for Model I (Tables 1 and 3) contain vertex points (the points of support for Scheffé's linear canonical polynomial (4)) edge points clustered about the vertices (apparently included to reflect the "edge" terms in x_i^{-1}), and a center point. In a similar manner the designs for Model II (Tables 2 and 4) contain vertex points and midpoints of q-2 edges (the points of support for Scheffe's quadratic canonical polynomial (5) and clusters of points, both edge and internal, near the vertices (apparently included to reflect the "edge" terms in x_i^{-1}). These designs were all obtained using Fedorov's D-optimality algorithm, as outlined above, and a grid-search on $\mathcal{X}_1$, to find the maximum of $d(\underline{x},\xi_i)$. The single-point exchange algorithm outlined above was also used to obtain exact designs in three and four components for Models I and II Some of these designs are given in Draper and St. John (1977b).

The present paper gives designs in five and six components for Models I and II. However, they were not obtained from a straightforward application

TABLE 1

Measure Design for Model I $(q = 3)$

Typical point in point set of support	No. of points in set	ξ^*	ξ_1	ξ_2
(.05,.05,.9)	3	.0871	.1	2/21
(.05,.17,.78)	6	.1011	.1	2/21
(1/3,1/3,1/3)	1		.1	
(.2,.2,.6)	3	.0440		1/21
$\lvert \underline{M}(\xi_i) \rvert$		121.5	118.0	120.5
$\max_{\mathcal{X}_1} d(\underline{x},\xi_i)$		6.03	6.24	6.19

TABLE 2

Measure Designs for Model II $(q = 3)$

Typical point in point set of support	No. of points in set	ξ^*	ξ_1
(.05,.05,.9)	3	.1015	1/9
(.05,.475,.475)	3	.1064	1/9
(.14,.14,.72)	3	.0940	1/9
(.05,.13,.82)	6	.0157	
$\lvert \underline{M}(\xi) \rvert$		$.715 \times 10^{-7}$	$.706 \times 10^{-7}$
$\max_{\mathcal{X}_1} d(\underline{x},\xi)$		9.03	9.51

TABLE 3

Measure designs for model I ($q = 4$)

Typical point in point sets of support	No. of points in set	ξ^*	ξ_1	ξ_2
(.05, .05, .14, .76)	12	.0722	.0730	1/14
(1/4, 1/4, 1/4, 1/4)	1	.1236	.1240	2/14
(.05, .05, .05, .85)	4	.0025		
$\lvert \underline{M}(\xi) \rvert$		94.59	94.53	93.42
$\max_{\mathcal{X}_1} d(\underline{x},\xi)$		8.01	8.12	8.17

TABLE 4

Measure designs for model II ($q = 4$)

Typical point in point sets of support	No. of points in set	ξ^*	ξ_1	ξ_2
(.05, .05, .05, .85)	4	.0652	.0662	.0670
(.05, .05, .45, .45)	6	.0541	.0658	.0638
(.05, .13, .13, .69)	12	.0176	.0202	
(.13, .13, .13, .61)	4	.0194		
(.05, .11, .42, .42)	12	.0105		
(.135, .135, .135, .595)	4		.0245	
(.05, .14, .14, .67)	12			.0291
$\lvert \underline{M}(\xi) \rvert$ (all times 10^{-17})		.2747	.2604	.2326
$\max_{\mathcal{X}_1} d(\underline{x},\xi)$		14.04	14.80	16.60

of the previously-outlined algorithms. We used recent improvements to Fedorov's algorithm and the symmetry of the models and design region to shorten what would otherwise have been a very expensive and time consuming process. We first discuss some of these improvements, and then give the designs.

2. ATWOOD'S IMPROVED D-OPTIMALITY ALGORITHM

Atwood (1973) presented three improvements to Fedorov's algorithm:

1. The maximum measure for any point of support of ξ^*, the D-optimal design, is $1/p$. If at any stage in the algorithm the measure at a design point is greater than $1/p$, allocate the excess measure uniformly to the other points in the design.

2. It may be possible to achieve a greater increase in the value of the determinant by <u>removing</u> measure from a point already in the design ξ_i and distributing the excess measure uniformly among the remaining points in design ξ_i. The point $\underline{x}_k$ from which measure is tentatively to be removed is given by finding $\underline{x}_k$ from the points of support of the current design ξ_i such that:

$$d(\underline{x}_k, \xi_i) = \min_{\{\underline{x}_j | \xi(\underline{x}_j) > 0\}} d(\underline{x}_j, \xi_i). \tag{11}$$

From Fedorov's algorithm we have that the point to which measure is tentatively to be added is given by finding $\underline{x}_i$ such that

$$d(\underline{x}_i, \xi_i) = \max_{\underline{x} \in \mathcal{X}} d(\underline{x}, \xi_i) \tag{12}$$

A comparison of the improvement to $|\underline{M}(\xi_i)|$ obtained by both actions leads to choice of the action that gives the greater increase in $|\underline{M}(\xi_i)|$.

3. In the event that several different actions (for example, adding measure to a point of maximum variance or removing measure from a design point of minimum variance) would lead to identical increases in the value of $|M(\xi_i)|$, choose the new design to be the equal-proportion convex combination of these potential designs. This convex combination design will be at least as good as any one of the potential designs.

Comments.

1. Atwood's first suggestion is based on his theorem (p. 343) stating that ξ^*, the D-optimal design, can have no point of support with measure greater than $1/p$. The point of support $\underline{x}_1$ from which measure is to be removed in order to reduce the measure at $\underline{x}_1$ to $1/p$ may also correspond to the design point with minimum variance, and therefore measure would possible be removed from $\underline{x}_1$ in any case. However, Atwood's procedure could be useful if the search for the point of minimum variance is expensive or time consuming.

2. Atwood's second suggestion is an excellent one. Tsay (1976) gives a related suggestion. We present the details of this procedure, and then discuss a possible improvement to Atwood's result. Suppose the current design is denoted by ξ_i, the single-point design at $\underline{x}$ by $\varepsilon_{\underline{x}}$, the measure to be placed on $\varepsilon_{\underline{x}}$ by α_i and the updated design by $\xi_{i+1} = (1-\alpha_i)\xi_i + \alpha_i\varepsilon_{\underline{x}}$. Fedorov assumed that α_i is positive and developed his algorithm accordingly. Atwood points out that ξ_{i+1} is also a probability measure design when α_i is negative provided point $\underline{x}$ is a point of support of design ξ_i. Let $\beta_i = \alpha_i/(1-\alpha_i)$ then

$$\frac{|\underline{M}(\xi_{i+1})}{M(\xi_i)} = (1+\beta_i)^{-p}\ (1+\beta_i d(\underline{x},\xi_i)). \tag{13}$$

The derivative of the logarithm of (13) has a zero at

$$\beta_i(\underline{x}) = [d(\underline{x},\xi_i) - p][(p-1)d(\underline{x},\xi_i)]^{-1}. \tag{14}$$

The value of (13) for $\beta_i(x)$ in (14) is thus

$$[d(\underline{x},\xi_i)/p]^p[(p-1)/(d(\underline{x},\xi_i)-1)]^{p-1} \tag{15}$$

Now if $d(\underline{x},\xi_i) > p$, (15) is strictly increasing in $d(\underline{x},\xi_i)$, and if $d(\underline{x},\xi_i) < p$, (15) is strictly decreasing in $d(\underline{x},\xi_i)$. Therefore, Atwood suggests, find $\underline{x}_0$ to maximize $d(\underline{x},\xi_i)$ and $\underline{x}_1$ (where $\underline{x}_1$ is a point of support of ξ_i) to minimize $d(\underline{x},\xi_i)$, adding measure $\underline{x}_0$ or subtracting measure from $\underline{x}_1$ according to whichever gives greater value to (15). In either case

$\alpha_i = \beta_i/(1+\beta_i)$, and the new design is given by $\xi_{i+1} = (1-\alpha_i)\xi_i + \alpha_i \varepsilon_{\underline{x}}$. In addition, Fedorov's method of updating $\underline{M}(\xi_{i+1})$ and $\underline{M}^{-1}(\xi_{i+1})$ still holds. Atwood gives a simple proof that this modified algorithm converges to ξ^*.

This procedure is based on that part of the general equivalence theorem which implies that $d(\underline{x},\xi^*) = p$ at all points of support of the D-optimal design. This suggests that, when $d(\underline{x}_1,\xi_i) < p$, the measure removed from $\underline{x}_1$ should only be distributed among those points of support for which $d(\underline{x},\xi_i) > p$, and, in addition, the amount of measure given to such points should depend on the value of $d(\underline{x},\xi_i) - p$. That is, those points of support with largest variance should receive the excess removed from points of support with smallest variance, and the amount given should be proportional to the need (we might think of this as socialism for design of experiments). However, this method of distributing the excess measure no longer allows use of Fedorov's simple method of updating $\underline{M}(\xi_{i+1})$ and $\underline{M}^{-1}(\xi_{i+1})$. We shall discuss our use of this procedure in detail in Section 3.

3. Atwood's third suggestion is also a very good one but can be improved. Suppose we assume that m ties occur only when the "tied" designs $\xi_{i+1,1}$, $\xi_{i+1,2}$, ..., $\xi_{i+1,m}$ all represent adding measure to a point, or all represent removing measure from a point of support. Then Atwood's suggestion that we let $\xi_{i+1} = \frac{1}{m}\sum_{j=1}^{m} \xi_{i+1,j}$ is not the optimal solution. Suppose the m proposed designs are all designs which add measure to corresponding points. The new design ξ_{i+1} obtained by adding measure α_i/m to each of the m points of maximum $d(\underline{x},\xi_i)$ is

$$\xi_{i+1} = (1-\alpha_i)\xi_i + (\alpha_i/m)\varepsilon_m, \tag{16}$$

where ε_m represents the m-point design concentrated on the points of maximum $d(\underline{x},\xi_i)$. Let the p x m matrix $\underline{F}$ be

$$\underline{F} = \begin{bmatrix} f_1(\underline{x}_1) & \cdots & f_1(\underline{x}_m) \\ f_2(\underline{x}_1) & & f_2(\underline{x}_m) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ f_p(\underline{x}_1) & \cdots & f_p(\underline{x}_m) \end{bmatrix} \qquad (17)$$

Then

$$\begin{aligned} \underline{M}(\xi_{i+1}) &= (1-\alpha_i)\underline{M}(\xi_i) + \alpha_i/m \;\; \underline{F}\,\underline{F}', \\ &= (1-\alpha_i)\{\underline{M}(\xi_i) + \left[\frac{\alpha_i/m}{1-\alpha_i}\right] \underline{F}\,\underline{F}'\}\,, \\ &= (1-\alpha_i)\{\underline{M}(\xi_i) + \underline{G}\,\underline{G}'\}, \qquad (18) \end{aligned}$$

where $$\underline{G} = \left[\frac{\alpha_i/m}{1-\alpha_i}\right]^{1/2} \underline{F}.$$

Therefore

$$|\underline{M}(\xi_{i+1})| = (1-\alpha_i)^p |\underline{I}_m + \underline{G}'\underline{M}^{-1}(\xi_i)\underline{G}|\;|\underline{M}(\xi_i)|, \quad (19)$$

and

$$\frac{|\underline{M}(\xi_{i+1})|}{|\underline{M}(\xi_i)|} = (1-\alpha_i)^p |\underline{I}_m + \frac{\alpha_i/m}{1-\alpha_i}\;\; \underline{F}'\underline{M}^{-1}(\xi_i)\underline{F}|, \quad (20)$$

where $\underline{I}_m$ is the $m \times m$ identity matrix. When $m = 1$, (20) corresponds to (13). When $m > 1$, the optimal solution to (20) is obtained by maximizing (20) with respect to α_i. An analytic solution to this maximization is difficult to obtain because α_i is contained within the determinant of an $m \times m$ matrix. However, we know that a solution must exist since Atwood's selection

$$\alpha_i = \left[\frac{\max_{\mathcal{X}} d(\underline{x},\xi_i) - p}{p(\max_{\mathcal{X}} d(\underline{x},\xi_i)-1)} \right] \qquad (21)$$

ensures at least one value of α_i (which may or may not be best) which quarantees that $|\underline{M}(\xi_{i+1})|/|\underline{M}(\xi_i)| \geq 1$. The range on α_i is $0 \leq \alpha_i \leq \min(m/p,1)$. We are unable (to date) to determine whether or not α_i has a unique turning point over this range. There exist a number of computer routines for obtaining a solution for α_i which maximizes (20). (Newton-Raphson type routines, for example).

Example 1 To illustrate the improvement that can be made in the selection of α_i when ties occur, we give this example. Suppose we wish to fit Model I:

$$E(y) = \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \beta_{-i} x_i^{-1},$$

and the design region is $\mathcal{X}_1 = \{\underline{x} \mid x_i \geq .05,\ i = 1,2,3;\ \sum_1^3 x_i = 1\}$. Assume the current design ξ_i has points of support (.05, .05, .9), (.05, .9, .05), (.9, .05, .05), $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, (.2, .2, .6), (.2,.6,.2) and (.6,.2, .2), each with equal measure of $\frac{1}{7}$. The value of $|\underline{M}(\xi_i)|$ is 5.12 and $\max_{\mathcal{X}_1} d(\underline{x},\xi_i) = 23.05$ is attained at each of the six points (.05, .17, .78), (.05, .78, .17), (.17, .05, .78), (.17, .78, .05), (.78, .05, .17) and (.78, .17, .05). Adding only one of these six points to design ξ_i would yield $\alpha_i = .1289$ and $|\underline{M}(\xi_{i+1})| = 9.88$. Adding all six points, each with measure $\alpha_i/6 = .0215$ would give $|\underline{M}(\xi_{i+1})| = 21.57$. This represents a considerable improvement over adding just one of the six points, but we can do even better. Table 5 gives the value of $|\underline{M}(\xi_{i+1})|$ for various values of $\alpha_i/6$. It is clear from this table that $\alpha_i/6 = .1142$ is a better value than $\alpha_i/6 = .0215$, providing a much larger value of $|\underline{M}(\xi_{i+1})|$.

Table 5

Values of $|\underline{M}(\xi_{i+1})|$ for Various Values of $\alpha_i/6$ for Example 1

$\alpha_i/6$	$\lvert\underline{M}(\xi_{i+1})\rvert$
.0208	20.89
.0215	21.57
.0267	26.93
.0325	33.29
.0383	40.03
.0442	47.32
.0500	54.54
.0558	61.81
.0617	69.33
.0675	76.37
.0733	83.06
.0792	89.63
.0850	95.90
.0908	99.98
.0967	104.17
.1025	106.84
.1083	108.15
.1142	108.31
.1165	107.65

3. SYMMETRY, GRID SEARCH, AND A DOUBLE ITERATION ALGORITHM

Symmetry We make the following assumptions which allow the use of a simplified procedure for obtaining approximately (to within acceptable numerical accuracy) D-optimal designs in five and six components:

1. The design region is symmetric about its centroid.
2. The model is symmetric in the variables.
3. There exists a D-optimal design which contains only point sets which are symmetric about the centroid of the design region.
4. Each point in a point set has the same measure.

The first two assumptions are satisfied for a number of design problems and in particular, by the mixture design problems we are considering. The third and fourth assumptions are satisfied by all of the D-optimal (to within acceptable numerical accuracy) measure designs previously obtained in three and four components (see Section 1)

Reducing the Number of Grid Points. We recall that, for three- and four-component mixtures, we searched the entire design region

$$\mathcal{X}_1 = \{\underline{x} | x_i \geq .05,\ i = 1,2, \ldots, q;\ \sum_1^q x_i = 1\}$$

in steps of size 0.01 to find $\max_{\mathcal{X}_1} d(\underline{x}, \xi_i)$. Such a method is not appropriate for five and six components because grid sizes of .04 or .05 are needed to keep the number of grid points reasonably low (because of computing cost) and then such a coarse grid might possibly yield designs which were far from best.

We note that under our assumptions 1 through 4, and the additional assumption that every intermediate design ξ_i is symmetric about the centroid of the design region, then the region

$$\mathcal{X}^* = \{\underline{x} \mid x_i \geq .05,\ i = 1, 2, \ldots, q;$$

$$x_j \geq x_i,\ j > i = 1, 2, \ldots, q-1;\ j = 2, 3, \ldots, q;\ \sum_1^q x_i = 1\} \tag{22}$$

will give the same solution to $\max_{\mathcal{X}^*} d(\underline{x}, \xi_i)$ as would be obtained from $\max_{\mathcal{X}_1} d(\underline{x}, \xi_i)$. By the "same solution" we mean that the two point sets generated by the two solutions will be identical. Now the number of grid points in $\mathcal{X}^*$ is $\prod_{i=0}^{q-2} 1/(q-i)$ times the number of grid points in $\mathcal{X}_1$, assuming the same grid size for both spaces. Therefore, for $q = 5$ and a grid size of 0.02 the number of grid points to be searched is reduced from 101,270 to approximately 900 (we say "approximately" because we overlap slightly at the $x_j \geq x_i$ boundary in order to ensure full coverage). For $q = 6$ a reduction from 575,757 to approximately 850 points is achieved. Whenever $\max_{\mathcal{X}_1} d(\underline{x}, \xi_i)$ is to be evaluated, we need only evaluate $\max_{\mathcal{X}^*} d(\underline{x}, \xi_i)$.

<ins>A Double-Iteration Algorithm</ins> We shall assume, in addition to the above, that a design in $(q-1)$ components can be extended to give a reasonable tentative starting design in q components. Given this starting design, we optimize the design measure over the initial points of support and augment or reduce the points of support. The steps are as follows:

1. Calculate $d(\underline{x}, \xi_i)$ at one point selected from each point set.

2. If $d(\underline{x}, \xi_i)$ at a point is less than p, remove measure from each point in the corresponding point set; if $d(\underline{x}, \xi_i)$ at a point is greater than p, add measure to each point in the corresponding point set. Recall that the average value over the points of support of $d(\underline{x}, \xi_i)$ is p, and therefore if $d(\underline{x}, \xi_i) < p$ for some point, then $d(\underline{x}, \xi_i) > p$ for some other point. Repeat steps 1 and 2 until $d(\underline{x}, \xi_i) \approx p$ at all points of support.

3. Calculate $d(\underline{x},\xi_i)$ for various neighbors of the points of support. For example, if the point of support is (.05, .05, .14, .71), calculate $d(\underline{x},\xi_i)$ for (.05, .05, .13, .72) and for (.05, .05, .15, .70). If $d(x,\xi_i)>p$ for one of these neighbors, shift the point set of support in that direction and repeat steps 1 and 2 above.

4. Given a tentatively D-optimal design from steps 2 and 3, find max $d(\underline{x},\xi_i)$, If max $d(\underline{x},\xi_i)$ is acceptably close to p (that is, max $d(\underline{x},\xi_i) \leq p + .05$), the design is approximately D-optimal. If max $d(\underline{x},\xi_i) > p + .05$, add to the proposed design the point set corresponding to the point at which this maximum occurs and return to step 1.

Example 2. Suppose we wish to obtain a D-optimal design for Model I, equation (6), in five components. The design region is $\mathcal{X}_1$. From the D-optimal design in four components (see Table 3), we suggest that a tentative design in five components have the twenty-one points of support consisting of (.2, .2, .2, .2, .2) and the twenty coordinate combinations of (.05,.05, .05, .14, .71). The design with equal measure of 0.0476 at each point of support has $|\underline{M}(\xi_i)| = 21.37$ and $d(\underline{x},\xi_i) = 21.00$ at (.2, .2, .2, .2, .2) and $d(\underline{x},\xi_i) = 9.45$ at (.05, .05, .05, .14, .71). One iteration of Fedorov's algorithm gives the design with measure 0.10 at (.2, .2, .2, .2, .2) and 0.0450 at each of the twenty points of the form (.05, .05, .05, .14, .71) with $|\underline{M}(\xi_i)| = 26.97$. The value of $d(\underline{x},\xi_i)$ for various neighboring points is given in Table 6. Note that $d(\underline{x},\xi_i) \simeq p$ (within two decimal places) for the points of support of this twenty-one point design, and therefore that this is the approximately optimal measure on this twenty-one point design.

The next step is to find $\max_{\mathcal{X}^*} d(\underline{x},\xi_i)$ for this design. A grid search through $\mathcal{X}^*$ in steps of size 0.02 gives the value $\max_{\mathcal{X}^*} d(\underline{x},\xi_i) = 10.74$ at (.05,.25, .24, .23, .23). We assume that the true maximum lies at the point (.05, .2375, .2375, .2375, .2375) and we add the corresponding five-point

Table 6

Values of $d(\underline{x},\xi_i)$ for Various Selected Neighbors of the 21 Points of Support of a Certain Design

$d(\underline{x},\xi_i)$	Points
9.97	(.05, .05, .05, .13, .72)
10.00	(.05, .05, .05, .14, .71)
9.99	(.05, .05, .05, .15, .70)
10.00	(.2, .2, .2, .2, .2)
9.99	(.2, .2, .2, .21, .19)

Table 7

Values of $\alpha_i/5$ and the Corresponding Values of $|\underline{M}(\xi_{i+1})|$ When Adding a Five-Point Set to the Current Design

$\alpha_i/5$	$\lvert\underline{M}(\xi_{i+1})\rvert$
.0010	27.06
.0015	27.10
.0025	27.16
.0035	27.22
.0045	27.27
.0055	27.31
.0065	27.26

point set to the twenty-one current points of support. If we were to add the single point (.05, .2375, .2375, .2375, .2375) to the twenty-one point design, the appropriate value of α_i would be .0076. Atwood's suggestion for $\alpha_i/5$ when adding all five points is to take $\alpha_i/5 = .0076/5 \simeq 0.0015$. Various values of $\alpha_i/5$ and the resulting values of $|\underline{M}(\xi_{i+1})|$ are given in Table 7. We shall use the slightly better value $\alpha_i/5 = 0.0055$ here to give design ξ_{i+1} with measure 0.0965 at (.2, .2, .2, .2, .2), 0.0438 at each of the twenty points of the form (.05, .05, .05, .14, .71), and 0.0055 at each of the five points of the form (.05, .2375, .2375, .2375, .2375). The values of $d(\underline{x},\xi_{i+1})$ for the three types of point of support is given in Table 8. Because $d(\underline{x},\xi_{i+1}) = 9.01 < p = 10$ at (.2, .2, .2, .2, .2), we remove measure from this point and distribute the measure among the five points of the form (.05, .2375, .2375, .2375, .2375), which have $d(\underline{x},\xi_{i+1}) = 10.15 > p = 10$. The sequence of designs generated in this manner is displayed in Table 8. Design ξ_{i+17} is the approximately D-optimal design <u>on these 26 points of support</u>. The neighbors of the 26 points of support also have values of $d(\underline{x},\xi_{i+17})$ very close to p, which indicates that the points of support cannot be shifted slightly to improve the design. A grid search of $\mathcal{X}^*$ using a grid size of 0.02 gives a maximum value of $d(\underline{x},\xi_{i+17}) = 10.03$, so that ξ_{i+17} is an approximately D-optimal design.

The D-optimal design for this example could have been obtained by a direct application of Fedorov's algorithm. However for models with more than ten parameters, the computational expense of doing this would be very high. For this example, our alternative procedure required only <u>two</u> searches of $\mathcal{X}^*$ to find the maximum value of $d(\underline{x},\xi_i)$, and so was comparatively efficient from the computing aspect.

Table 8

Design Sequence for Model I (q = 5)

Design		Point Sets of Support			
		(.2, .2, .2, .2, .2)	(.05, .05, .05, .14, .71)	(.05, .2375, .2375, .2375, .2375)	$\|M(\xi)\|$
ξ_{i+1}	Measure	.0965	.0438	.0055	27.31
	$d(\underline{x},\xi_{i+1})$	9.01	10.11	10.15	
ξ_{i+2}	Measure	.0900	.0438	.0068	27.49
	$d(\underline{x},\xi_{i+2})$	9.26	10.07	10.23	
ξ_{i+3}	Measure	.0800	.0438	.0088	27.72
	$d(\underline{x},\xi_{i+3})$	9.69	10.00	10.38	
ξ_{i+4}	Measure	.0700	.0438	.0108	27.87
	$d(\underline{x},\xi_{i+4})$	10.15	9.95	10.56	
ξ_{i+5}	Measure	.0700	.0428	.0148	28.02
	$d(\underline{x},\xi_{i+5})$	9.18	10.07	10.00	
ξ_{i+6}	Measure	.0600	.0433	.0148	28.12
	$d(\underline{x},\xi_{i+6})$	10.10	9.96	10.43	
ξ_{i+7}	Measure	.0600	.0428	.0168	28.21
	$d(\underline{x},\xi_{i+7})$	9.60	10.01	10.14	
ξ_{i+8}	Measure	.0500	.0428	.0188	28.32
	$d(\underline{x},\xi_{i+8})$	10.06	9.96	10.31	
ξ_{i+9}	Measure	.0500	.0418	.0228	28.33
	$d(\underline{x},\xi_{i+9})$	9.11	10.08	9.78	
ξ_{i+10}	Measure	.0400	.0423	.0228	28.46
	$d(\underline{x},\xi_{i+10})$	10.02	9.97	10.20	
ξ_{i+11}	Measure	.04	.0420	.0240	28.49
	$d(\underline{x},\xi_{i+11})$	9.71	10.01	10.03	
ξ_{i+12}	Measure	.03	.0420	.0260	28.53
	$d(\underline{x},\xi_{i+12})$	10.19	9.96	10.21	
ξ_{i+13}	Measure	.03	.0416	.0276	28.56
	$d(\underline{x},\xi_{i+13})$	9.78	10.01	9.98	
ξ_{i+14}	Measure	.0280	.0417	.0276	28.57
	$d(\underline{x},\xi_{i+14})$	9.97	9.99	10.07	
ξ_{i+15}	Measure	.0270	.0416	.0282	28.57
	$d(\underline{x},\xi_{i+15})$	9.92	10.00	10.03	
ξ_{i+16}	Measure	.0260	.0416	.0284	28.58
	$d(\underline{x},\xi_{i+16})$	9.97	9.99	10.05	
ξ_{i+17}	Measure	.0240	.0415	.0292	28.58
	$d(\underline{x},\xi_{i+17})$	10.00	10.00	10.03	

It is possible that D-optimal designs with fewer than twenty-six points of support exist. In general, the procedure which we have outlined will not necessarily give the most parsimonious design (that is, the design with fewest points of support). For this reason we have tried, while applying our procedure, to remove point sets from the points of support whenever possible. However we are uncertain if this results in a more parsimonious design. We know that there always exists at least one D-optimal design with at most $\binom{p}{2}$ points of support. All our designs have fewer than $\binom{p}{2}$ points of support.

4. MEASURE DESIGNS IN FIVE AND SIX COMPONENTS

<u>Five Components</u> The approximately D-optimal design ξ^* on region $\mathcal{X}_1$ for Model I is given in Table 9. We discussed the method of obtaining this design in our example of Section 3. Design ξ_1 is a simple extension of the D-optimal design in four components (see Table 3), the vertex points with small measure having been dropped. Design ξ^* splits the center point of design ξ_1 and distributes measure among these five new points. Either design ξ_1 or ξ^* would form a good base for developing exact n-point designs for this model.

Table 9

Measure Designs for Model I (q = 5)

Point Sets of Support	No. of Points in Set	ξ^*	ξ_1
(.2, .2, .2, .2, .2)	1	.0240	.1000
(.05, .2375, .2375, .2375, .2375)	5	.0292	
(.05, .05, .05, .14, .71)	20	.0415	.0450
$\lvert \underline{M}(\xi) \rvert$		28.58	26.97
$\max_{\mathcal{X}_1} d(\underline{x},\xi)$		10.03	10.74

The approximately D-optimal design ξ^* on region $\mathcal{X}_1$ for model II is given in Table 10. ξ^* gives largest measure to the points of support of the second order canonical polynomial, that is, points of the form (.05, .05, .05, .05, .80) and (.05, .05, .05, .425, .425), as was the case for the design in four components. However, where the four component design contained three types of point sets to yield estimates of the inverse terms (see Table 4), ξ^* contains only two types of point sets for this purpose. Specifically, the point sets of the form

(.05, .05, .1, .4, .4) and (.05, .12, .12, .12, .59) in design ξ^* are apparently included to provide estimates of the inverse terms, the former being the extension of the point set of the form (.05, .11, .42, .42) in four components, and the latter being the extension of the point sets of the form (.05, .13, .13, .69) and (.13, .13, .13, .61).

Table 10

Measure Designs for Model II (q = 5)

Point Sets of Support	No. of Points in Set	ξ^*	ξ_1
(.05, .05, .05, .05, .8)	5	.0476	.0484
(.05, .05, .05, .425, .425)	10	.0316	.0464
(.05, .12, .12, .12, .59)	20	.0109	.0147
(.05, .05, .1, .4, .4)	30	.0076	
$\lvert \underline{M}(\xi) \rvert$		$.8530 \times 10^{-33}$	$.7511 \times 10^{-33}$
$\max_{\mathcal{X}_1} d(\underline{x},\xi)$		20.07	21.07

Design ξ_1 is not D-optimal. However, because it has fewer points of support and yet has a comparatively large value of $\lvert \underline{M}(\xi_1) \rvert$, this design would probably make a better starting point for obtaining exact n-point designs.

Six Components The approximately D-optimal design on region $\mathcal{X}_1$ for model I is given in Table 11. The design contains central point sets of the form (.05, .05, .225, .225, .225, .225) and (.05, .19, .19, .19, .19, .19), which are apparently extensions of point sets of the form (.2, .2, .2, .2, .2)

and (.05, .2375, .2375, .2375, .2375) for the design in five components. The point set of the form (.05, .05, .05, .14, .71) in five components has split to give the two points sets of the form (.05, .05, .05, .05, .12, .68) and (.05, .05, .05, .13, .13, .69) in six components.

The design ξ_1 is nearly D-optimal and has fifty-one points of support, whereas ξ^* has one hundred and eleven points of support. Thus design ξ_1 might form a better base for obtaining exact n-point designs.

Table 11

Measure Designs for Model I (q = 6)

Point Sets of Support	No. of Points in Set	ξ^*	ξ_1
(.05, .05, .05, .05, .12, .68)	30	.0223	.02505
(.05, .19, .19, .19, .19, .19)	6	.0102	.00644
(.05, .05, .225, .225, .225, .225)	15	.0100	.01399
(.05, .05, .05, .13, .13, .59)	60	.0020	
$\lvert \underline{M}(\xi) \rvert$		3.92	3.87
$\max_{\mathcal{X}_1} d(\underline{x},\xi)$		12.02	12.13

Table 12 contains the approximately D-optimal design on region $\mathcal{X}_1$ for model II. As was the case for the approximately D-optimal design in five components, ξ^* places largest measure on the points of support of the second order canonical polynomial, that is, the point sets of the form (.05, .05, .05, .05, .05, .75) and (.05, .05, .05, .05, .4, .4). The other three point sets in ξ^* are apparently introduced for estimating inverse terms, and these three point sets are similar to the two point sets of the form (.05, .05, .1, .4, .4)

and (.05, .12, .12, .12, .59) contained in the five-component approximately D-optimal design (see Table 10).

Design ξ^* contains 171 points of support, a number which is quite large for implementing exact n-point designs. Design ξ_1 is very nearly D-optimal, and has 30 fewer points of support than does ξ^*. Also, design ξ_2 has only 81 points of support but still has a very large value of $|\underline{M}(\xi_2)|$, relative to the value of $|\underline{M}(\xi^*)|$. Thus design ξ_2 might probably be preferable to ξ^* and ξ_1 for use as a base for obtaining an exact n-point design. We also note that ξ_1 is the design obtained when the points of minimum measure are dropped from ξ^* and distributed among the remaining points of support so as to maximize $|M(\xi_1)|$. Similarly ξ_2 is the design obtained when the points of minimum measure are dropped from ξ_1.

Table 12

Measure Designs for Model II (q = 6)

Point Sets of Support	No. of Points in Set	ξ^*	ξ_1	ξ_2
(.05, .05, .05, .05, .05, .75)	6	.03551	.03544	.03567
(.05, .05, .05, .05, .4, .4)	15	.02398	.02469	.03400
(.05, .05, .12, .12, .12, .54)	60	.00357	.00365	.00460
(.05, .05, .05, .09, .38, .38)	60	.00326	.00330	
(.05, .12, .12, .12, .12, .47)	30	.00058		
$\lvert\underline{M}(\xi)\rvert$		$.4832\times10^{-54}$	$.4817\times10^{-54}$	$.4458\times10^{-54}$
$\max_{x} d(\underline{x},\xi)$		27.08	27.40	27.75

5. EXACT DESIGNS IN FIVE AND SIX COMPONENTS

Five Components We shall give exact n-point designs which are sequentially optimal and n-point designs which are D_n-optimal. The sequentially optimal designs are developed by first finding the D_n-optimal design for $n = p$, and then sequentially adding the candidate point with maximum variance to the n-point design to obtain the $(n+1)$-point design. Because these sequential designs are not necessarily D_n-optimal, we used these sequential designs as starting designs and employed Fedorov's single-point-exchange algorithm to obtain D_n-optimal designs. The D_n-optimal designs are given only when they differ from the sequentially optimal designs.

The major drawback in obtaining designs in five and six components is the cost of computing variances, which involves quadratic forms with matrices of dimension $p \times p$ over a large number of candidate points. For this reason we shall limit the set of candidate points for exact designs to the set of points of support of the corresponding measure designs.

When the number of points of support is quite large (65 for model II in five components, for example) we will also obtain exact designs using the points of support of near-optimal designs (there being fewer points of support for such designs) as the set of candidate points. In this way, we hope to determine if good designs can be obtained using fewer points of support. We note that restricting the set of candidate points in this manner will necessarily give sub-optimal designs for n small and close to the number of parameters (the designs are sub-optimal relative to the designs that could be obtained if the set of candidates were the entire set of points in design region $\mathcal{X}_1$). However, as n gets larger, the sequence of exact designs will converge to the approximately D-optimal design ξ^*. We shall also use this procedure of selecting candidate points for exact designs in six components.

Table 13 contains sequentially optimal designs for model I for $n = 10$ through $n = 22$. The set of candidate points for these designs is the set of 26 points of support of the corresponding measure design ξ^* in Table 9. We note that the designs for small n ($n = 10, 11, 12, 13$) have very low values of $|\underline{M}(\xi(n))|$. Since this was not true for exact designs for model I in four components (see Draper and St. John (1977b)), where we did not restrict the set of candidate points to be the set of points of support of the measure design, we suggest that this low efficiency for small n may be largely due to this restriction. As n gets larger ($n = 19, 20, 21, 22$), these sequential designs improve to the point where $|\underline{M}(\xi(22))| = 26.83$, compared to the optimal value of 28.58.

Most of the sequential designs in Table 13 are also D_n-optimal; better designs were obtained only for $n = 12$, 18, and 19, as given in Table 14. We note that all three of these designs are similar to the sequential design; only one point was exchanged in each to obtain the D_n-optimal design. We also note that the D_n-optimal designs are only slightly better, in the value of $|\underline{M}(\xi(n))|$, than the sequentially optimal designs.

We obtained exact designs for model II using the thirty-five points of support of design ξ_1 in Table 10 as the set of candidates, and using the sixty-five points of support of design ξ^* in Table 10 as candidates. We shall first give the designs obtained using the thirty-five points of support.

Table 15 contains sequential designs from 35 candidates for model VI for $n = 20$ through 32. As was the case in four components, exact designs for model II in five components contain the D-optimal design points for the second order canonical polynomial with points added to estimate the inverse terms. As we also noted for the designs in four components, the value of $|\underline{M}(\xi(n))|$ does not increase very rapidly toward the optimal value of $.8530 \times 10^{-33}$.

Table 13

Sequential Designs for Model I (q = 5)

Point No.	Point	$\lvert\underline{M}(\xi(n))\rvert$
1	(.05, .05, .05, .14, .71)	
2	(.05, .05, .14, .05, .71)	
3	(.14, .05, .05, .71, .05)	
4	(.05, .14, .05, .71, .05)	
5	(.05, .05, .71, .05, .14)	
6	(.05, .05, .71, .14, .05)	
7	(.05, .71, .14, .05, .05)	
8	(.71, .14, .05, .05, .05)	
9	(.71, .05, .05, .05, .14)	
10	(.2, .2, .2, .2, .2)	.88
11	(.14, .71, .05, .05, .05)	3.39
12	(.05, .71, .05, .05, .14)	4.97
13	(.05, .14, .05, .05, .71)	7.66
14	(.14, .05, .71, .05, .05)	9.89
15	(.05, .05, .14, .71, .05)	11.75
16	(.71, .05, .05, .14, .05)	14.53
17	(.2, .2, .2, .2, .2)	15.84
18	(.71, .05, .14, .05, .05)	17.02
19	(.05, .14, .71, .05, .05)	18.87
20	(.05, .71, .05, .14, .05)	21.04
21	(.05, .05, .05, .71, .14)	23.50
22	(.14, .05, .05, .05, .71)	26.83

Table 14

Exact Designs for Model I (q = 5)

Design Points	No. of Points in Design 12	18	19
(.05, .05, .05, .14, .71)	1	1	1
(.05, .05, .14, .05, .71)	1	1	1
(.05, .14, .05, .05, .71)		1	1
(.14, .05, .05, .05, .71)			
(.05, .05, .05, .71, .14)			
(.05, .05, .14, .71, .05)	1	1	1
(.05, .14, .05, .71, .05)	1	1	1
(.14, .05, .05, .71, .05)	1	1	1
(.05, .05, .71, .05, .14)	1	1	1
(.05, .05, .71, .14, .05)	1	1	1
(.05, .14, .71, .05, .05)		1	1
(.14, .05, .71, .05, .05)		1	1
(.05, .71, .05, .05, .14)	1	1	1
(.05, .71, .05, .14, .05)			1
(.05, .71, .14, .05, .05)		1	1
(.14, .71, .05, .05, .05)	1	1	1
(.71, .05, .05, .05, .14)	1	1	1
(.71, .05, .05, .14, .05)		1	
(.71, .05, .14, .05, .05)		1	1
(.71, .14, .05, .05, .05)	1		1
(.2, .2, .2, .2, .2)	1	2	2
$\lvert \underline{M}(\xi(n)) \rvert$	5.54	17.39	19.29

Table 15

Sequential Designs for Model II ($q = 5$) From 35 Candidates

Point No.	Point	$\lvert \underline{M}(\xi(n)) \rvert$*
1	(.05, .05, .05, .05, .8)	
2	(.05, .05, .05, .8, .05)	
3	(.05, .05, .8, .05, .05)	
4	(.05, .8, .05, .05, .05)	
5	(.8, .05, .05, .05, .05)	
6	(.05, .05, .05, .425, .425)	
7	(.05, .05, .425, .05, .425)	
8	(.05, .425, .05, .05, .425)	
9	(.425, .05, .05, .05, .425)	
10	(.05, .05, .425, .425, .05)	
11	(.05, .425, .05, .425, .05)	
12	(.425, .05, .05, .425, .05)	
13	(.05, .425, .425, .05, .05)	
14	(.425, .05, .425, .05, .05)	
15	(.425, .425, .05, .05, .05)	
16	(.12, .05, .12, .12, .59)	
17	(.12, .12, .12, .59, .05)	
18	(.12, .05, .59, .12, .12)	
19	(.12, .59, .12, .05, .12)	
20	(.59, .05, .12, .12, .12)	.0980
21	(.05, .12, .59, .12, .12)	.2053
22	(.12, .12, .05, .59, .12)	.2374
23	(.12, .12, .05, .12, .59)	.2804
24	(.59, .12, .12, .05, .12)	.3194
25	(.59, .12, .12, .12, .05)	.3067
26	(.8, .05, .05, .05, .05)	.2767
27	(.05, .425, .05, .425, .05)	.2569
28	(.05, .8, .05, .05, .05)	.2444
29	(.05, .05, .8, .05, .05)	.2381
30	(.05, .05, .05, .8, .05)	.2376
31	(.05, .05, .05, .05, .8)	.2424
32	(.05, .05, .425, .05, .425)	.2492

* All times 10^{-33}

Table 16

Exact Designs for Model II (q = 5) From 35 Candidates

	No. of Points in Design										
	22	23	24	25	26	27	28	29	30	31	32
(.05, .05, .05, .05, .8)	1	1	1	1	1	1	2	2	2	2	2
(.05, .05, .05, .8, .05)	1	1	1	1	1	1	1	1	2	2	2
(.05, .05, .8, .05, .05)	1	1	1	1	1	2	1	2	2	2	2
(.05, .8, .05, .05, .05)	1	1	1	1	1	1	2	2	2	2	2
(.8, .05, .05, .05, .05)	1	1	1	1	2	2	2	2	2	2	2
(.05, .05, .05, .425, .425)	1	1	1	1	1	1	1	1	1	1	1
(.05, .05, .425, .05, .425)	1	1	1	1	1	1	1	1	1	1	2
(.05, .425, .05, .05, .425)	1	1	1	1	1	1	1	1	1	1	1
(.425, .05, .05, .05, .425)	1	1	1	1	1	1	1	1	1	1	1
(.05, .05, .425, .425, .05)	1	1	1	1	1	1	1	1	1	1	1
(.05, .425, .05, .425, .05)	1	1	1	1	1	1	1	1	1	1	1
(.425, .05, .05, .425, .05)	1	1	1	1	1	1	1	1	1	1	1
(.05, .425, .425, .05, .05)	1	1	1	1	1	1	1	1	1	1	2
(.425, .05, .425, .05, .05)	1	1	1	1	1	1	1	1	1	1	1
(.425, .425, .05, .05, .05)	1	1	1	1	1	1	1	1	1	2	1
(.12, .05, .12, .12, .59)			1	1	1	1	1	1	1	1	1
(.12, .12, .12, .59, .05)	1	1	1	1	1	1	1	1	1	1	1
(.12, .05, .59, .12, .12)	1	1	1	1	1	1	1	1	1	1	1
(.12, .59, .12, .05, .12)	1	1	1	1	1	1	1	1	1	1	1
(.59, .05, .12, .12, .12)	1	1									
(.05, .12, .59, .12, .12)	1	1	1	1	1	1	1	1	1	1	1
(.12, .12, .05, .59, .12)	1	1	1	1	1	1	1	1	1	1	1
(.12, .12, .05, .12, .59)	1	1	1	1	1	1	1	1	1	1	1
(.12, .59, .12, .12, .05)		1									
(.59, .12, .12, .05, .12)			1	1	1	1	1	1	1	1	1
(.05, .59, .12, .12, .12)			1	1	1	1	1	1	1	1	1
(.59, .12, .12, .12, .05)				1	1	1	1	1	1	1	1
$\lvert \underline{M}(\xi(n)) \rvert$ (All Times 10^{-33})	.2535	.2933	.3224	.3337	.2994	.2767	.2628	.2561	.2555	.2571	.2641

Table 17

Sequential Designs for Model II ($q = 5$) From 65 Candidates

Point No.	Point	$\lvert \underline{M}(\xi(n)) \rvert$*
1	(.05, .05, .05, .05, .8)	
2	(.05, .05, .05, .8, .05)	
3	(.05, .05, .8, .05, .05)	
4	(.05, .8, .05, .05, .05)	
5	(.8, .05, .05, .05, .05)	
6	(.05, .05, .05, .425, .425)	
7	(.05, .05, .425, .05, .425)	
8	(.05, .425, .05, .05, .425)	
9	(.425, .05, .05, .05, .425)	
10	(.05, .05, .425, .425, .05)	
11	(.05, .425, .05, .425, .05)	
12	(.425, .05, .05, .425, .05)	
13	(.425, .05, .425, .05, .05)	
14	(.425, .425, .05, .05, .05)	
15	(.05, .4, .4, .1, .05)	
16	(.12, .05, .12, .12, .59)	
17	(.12, .12, .12, .59, .05)	
18	(.12, .05, .59, .12, .12)	
19	(.12, .59, .12, .05, .12)	
20	(.59, .05, .12, .12, .12)	.0983
21	(.59, .12, .05, .12, .12)	.1926
22	(.12, .12, .59, .05, .12)	.2345
23	(.05, .12, .12, .12, .59)	.2640
24	(.05, .12, .12, .59, .12)	.2893
25	(.05, .425, .425, .05, .05)	.3098
26	(.12, .12, .05, .12, .59)	.3018
27	(.4, .1, .4, .05, .05)	.2874
28	(.05, .4, .05, .4, .1)	.2737
29	(.05, .8, .05, .05, .05)	.2667
30	(.05, .05, .05, .05, .8)	.2657
31	(.05, .05, .8, .05, .05)	.2702
32	(.8, .05, .05, .05, .05)	.2805

* All Times 10^{-33}

The D_n-optimal designs for model II from 35 candidates are different from the sequential designs for $n = 22$ through 32. These D_n-optimal designs are given in Table 16. We note that the values of $|\underline{M}(\xi(n))|$ are only slightly better than the corresponding values for the sequential designs.

Table 17 contains the sequentially optimal designs for model II for $n = 20$ through 32 using as candidates the sixty-five points of support of design ξ^* in Table 10. The twenty-point design is the D_n-optimal design, but because of the computing expense we have not obtained D_n-optimal designs for $n > 20$, although this could be done without difficulty. We note, for the designs in Table 17, that (i) the twenty point design is different in one point from the twenty point design in Table 15, (ii) the designs for $n = 21$, 22, 23, and 24 are slightly inferior to the corresponding designs in Table 15, (iii) the designs for $n = 25$ through 32 are superior to the corresponding designs in Table 15 (The designs for $n > 32$ should also be superior because the set of candidates for the design in Table 15 is a proper subset of the set of candidates for the designs in Table 17).

The value of $|\underline{M}(\xi^*)|$ is 0.8503×10^{-33}. This optimal value is not approached by any of the designs in Tables 15, 16, and 17. We have previously noted that exact designs for model II in four components are also relatively inefficient. As a result of our calculations, we see what appears to be a fundamental difficulty in general in obtaining exact designs. It appears that, when there are a large number of points of support (for example, 65 for model II for $q = 5$) of the approximately D-optimal design for the model considered, and when the measures on these points of support vary widely (for example, see Table 10 for model II for $q = 5$), it is difficult to obtain exact designs with relatively large values of $|\underline{M}(\xi(n))|$ compared to the D-optimal value $|\underline{M}(\xi^*)|$.

This difficulty will appear again in the $q = 6$ case which follows. It appears, from our experience, that the best way of finding good exact designs for a model with many parameters, when the corresponding measure design ξ^* has many points of support with widely different measures is the following:

1. Find the D_n-optimal design for $n = p$ using the set of points of support of ξ^* as the set of candidate points.

2. Generate sequentially optimal $(n+1)$ - point designs by adding the candidate point of maximum variance to the n-point design. Designs obtained using this method would appear to be better than designs obtained using Fedorov's exchange algorithm when the set of candidates is a subset of the set of points of support of ξ^*. We shall mention this again with regard to exact designs in six components.

<u>Six Components</u>. We give exact sequential designs for Models I and II, and exact D_n-optimal designs for model I. For model II we shall give the D_n-optimal design only for $n = p = 27$. D_n-optimal designs for model II for n 27 are computationally expensive.

The set of candidate points for the designs given in Tables 18 and 19 is the set of fifty-one points of support of design ξ_1 in Table 11. Table 18 contains sequentially optimal designs for $n = 12$ through 24. The value of $|\underline{M}(\xi(n))|$ is fairly small for small n and increases gradually as n gets larger, with $|\underline{M}(\xi(24))| = 1.91$ not very close to the D-optimal value of 3.92.

The D_n-optimal designs in Table 19 were obtained using the sequential designs in Table 18 as starting designs and applying Fedorov's point-exchange algorithm over the 51 candidates. No improvement was possible for $n = 12$ through $n = 18$. The D_n-optimal designs for $n = 19$ through 24 are given in Table 19.

We used the 111 points of support of the approximately D-optimal design ξ^* in Table 11 as the candidates for the designs given in Table 20. The twelve-point design is D_n-optimal and the designs for $n = 13$ through 24 are sequentially

Table 18

Sequential Designs for Model I (q = 6) From 51 Candidates

Point No.	Point	$\lvert \underline{M}(\xi(n)) \rvert$
1	(.05, .05, .05, .05, .12, .68)	
2	(.05, .05, .12, .05, .68, .05)	
3	(.05, .12, .05, .05, .68, .05)	
4	(.05, .05, .05, .68, .12, .05)	
5	(.12, .05, .05, .68, .05, .05)	
6	(.05, .05, .68, .05, .05, .12)	
7	(.05, .05, .68, .12, .05, .05)	
8	(.05, .68, .05, .05, .05, .12)	
9	(.68, .12, .05, .05, .05, .05)	
10	(.225, .05, .05, .225, .225, .225)	
11	(.225, .225, .225, .05, .225, .05)	
12	(.05, .225, .225, .225, .05, .225)	.228
13	(.68, .05, .12, .05, .05, .05)	.349
14	(.12, .05, .05, .05, .05, .68)	.573
15	(.05, .68, .05, .12, .05, .05)	1.00
16	(.05, .05, .05, .12, .68, .05)	.976
17	(.68, .05, .05, .05, .05, .12)	.995
18	(.19, .19, .19, .19, .05, .19)	1.05
19	(.12, .05, .68, .05, .05, .05)	1.14
20	(.05, .12, .05, .05, .05, .68)	1.27
21	(.05, .05, .12, .68, .05, .05)	1.44
22	(.05, .68, .05, .05, .12, .05)	1.59
23	(.05, .05, .225, .225, .225, .225)	1.74
24	(.225, .225, .05, .225, .225, .05)	1.91

Table 19

Exact Designs for Model I (q = 6) From 51 Candidates

Design Points	No. of Points in Design					
	19	20	21	22	23	24
(.05, .12, .05, .05, .05, .68)	1	1	1	1	1	1
(.12, .05, .05, .05, .05, .68)	1	1	1	1	1	1
(.05, .05, .05, .05, .12, .68)	1	1	1			
(.05, .05, .05, .12, .68, .05)	1	1	1	1		
(.05, .05, .12, .05, .68, .05)	1	1	1	1	1	1
(.05, .12, .05, .05, .68, .05)	1	1	1	1	1	1
(.05, .05, .12, .68, .05, .05)	1	1	1	1	1	1
(.05, .05, .05, .68, .12, .05)	1	1		1		
(.12, .05, .05, .68, .05, .05)	1	1		1	1	1
(.05, .05, .68, .05, .05, .12)	1	1	1	1	1	1
(.05, .05, .68, .12, .05, .05)	1	1	1	1	1	1
(.05, .68, .05, .12, .05, .05)	1	1	1	1	1	1
(.05, .68, .05, .05, .05, .12)	1	1	1	1	1	1
(.68, .05, .12, .05, .05, .05)	1	1	1	1		
(.68, .12, .05, .05, .05, .05)	1	1	1	1		
(.19, .19, .19, .19, .05, .19)	1	1	1	1		
(.05, .19, .19, .19, .19, .19)	1	1	1	1		
(.225, .05, .05, .225, .225, .225)	1	1	1	1	1	1
(.225, .225, .225, .05, .225, .05)	1	1	1	1	1	1
(.68, .05, .05, .05, .05, .12)		1	1	1	1	1
(.12, .05, .68, .05, .05, .05)			1	1		
(.05, .68, .05, .05, .12, .05)			1	1	1	1
(.05, .12, .05, .68, .05, .05)			1		1	1
(.05, .05, .12, .05, .05, .68)				1	1	1
(.05, .05, .225, .225, .225, .225)					1	1
(.225, .225, .225, .225, .05, .05)					1	1
(.05, .225, .05, .225, .225, .225)					1	1
(.225, .225, .225, .05, .05, .225)					1	1
(.05, .05, .68, .05, .12, .05)					1	1
(.12, .05, .05, .05, .68, .05)					1	1
(.68, .05, .05, .12, .05, .05)					1	1
(.68, .05, .05, .05, .12, .05)						1
$\lvert \underline{M}(\xi(n)) \rvert$	1.29	1.45	1.64	1.83	2.19	2.59

Table 20

Sequential Designs for Model I $(q = 6)$ From 111 Candidates

Point No.	Point	$\lvert \underline{M}(\xi(n)) \rvert$
1	(.05, .12, .05, .05, .68, .05)	
2	(.05, .59, .05, .13, .13, .05)	
3	(.225, .05, .05, .225, .225, .225)	
4	(.225, .225, .225, .05, .225, .05)	
5	(.05, .05, .12, .05, .68, .05)	
6	(.05, .05, .05, .68, .12, .05)	
7	(.13, .05, .59, .13, .05, .05)	
8	(.13, .59, .05, .05, .05, .13)	
9	(.05, .05, .59, .05, .13, .13)	
10	(.05, .05, .05, .05, .12, .68)	
11	(.68, .05, .05, .12, .05, .05)	
12	(.05, .225, .225, .225, .05, .225)	.434
13	(.05, .12, .68, .05, .05, .05)	.518
14	(.68, .05, .12, .05, .05, .05)	.659
15	(.12, .05, .05, .05, .05, .68)	.840
16	(.05, .05, .12, .68, .05, .05)	1.07
17	(.59, .13, .05, .05, .05, .13)	1.30
18	(.05, .68, .12, .05, .05, .05)	1.55
19	(.19, .19, .19, .19, .19, .05)	1.73
20	(.13, .13, .05, .5o, .n5, .05)	1.92
21	(.05, .13, .05, .13, .05, .59)	2.18
22	(.05, .05, .05, .13, .59, .13)	2.36
23	(.19, .19, .19, .05, .19, .19)	2.39
24	(.12, .05, .05, .05, .68, .05)	2.46

Table 21

Sequential Designs for Model II (q = 6) From 81 Candidates

Point No.	Point	$\vert \underline{M}(\xi(n)) \vert$
1	(.05, .05, .05, .05, .05, .75)	
2	(.05, .05, .05, .05, .75, .05)	
3	(.05, .05, .05, .75, .05, .05)	
4	(.05, .05, .75, .05, .05, .05)	
5	(.05, .75, .05, .05, .05, .05)	
6	(.75, .05, .05, .05, .05, .05)	
7	(.4, .4, .05, .05, .05, .05)	
8	(.4, .05, .4, .05, .05, .05)	
9	(.4, .05, .05, .4, .05, .05)	
10	(.4, .05, .05, .05, .4, .05)	
11	(.4, .05, .05, .05, .05, .4)	
12	(.05, .4, .4, .05, .05, .05)	
13	(.05, .4, .05, .4, .05, .05)	
14	(.05, .4, .05, .05, .4, .05)	
15	(.05, .4, .05, .05, .05, .4)	
16	(.05, .05, .4, .4, .05, .05)	
17	(.05, .05, .4, .05, .4, .05)	
18	(.05, .05, .4, .05, .05, .4)	
19	(.05, .05, .05, .4, .4, .05)	
20	(.05, .05, .05, .4, .05, .4)	
21	(.05, .05, .05, .05, .4, .4)	
22	(.54, .05, .05, .12, .12, .12)	
23	(.05, .12, .12, .54, .05, .12)	
24	(.05, .12, .12, .12, .05, .54)	
25	(.12, .05, .05, .12, .54, .12)	
26	(.12, .54, .12, .05, .12, .05)	
27	(.12, .12, .54, .05, .12, .05)	$.859 \times 10^{-55}$
28	(.12, .12, .05, .54, .05, .12)	$.867 \times 10^{-55}$
29	(.05, .05, .12, .54, .12, .12)	$.905 \times 10^{-55}$
30	(.12, .05, .12, .12, .05, .54)	$.958 \times 10^{-55}$
31	(.05, .12, .05, .12, .12, .54)	$.104 \times 10^{-54}$
32	(.05, .12, .12, .05, .54, .12)	$.101 \times 10^{-54}$
33	(.05, .54, .05, .12, .12, .12)	$.983 \times 10^{-55}$
34	(.54, .12, .12, .12, .05, .05)	$.923 \times 10^{-55}$
35	(.05, .12, .54, .12, .05, .12)	$.862 \times 10^{-55}$
36	(.05, .05, .05, .75, .05, .05)	$.790 \times 10^{-55}$
37	(.05, .05, .05, .05, .05, .75)	$.738 \times 10^{-55}$
38	(.05, .05, .75, .05, .05, .05)	$.702 \times 10^{-55}$
39	(.05, .75, .05, .05, .05, .05)	$.679 \times 10^{-55}$
40	(.05, .05, .05, .05, .75, .05)	$.669 \times 10^{-55}$
41	(.75, .05, .05, .05, .05, .05)	$.668 \times 10^{-55}$

Table 22

Sequential Designs for Model II (q = 6) From 141 Candidates

Point No.	Point	$\lvert \underline{M}(\xi(n)) \rvert$
1	(.05, .05, .05, .05, .05, .75)	
2	(.05, .05, .05, .05, .75, .05)	
3	(.05, .05, .05, .75, .05, .05)	
4	(.05, .05, .75, .05, .05, .05)	
5	(.05, .75, .05, .05, .05, .05)	
6	(.75, .05, .05, .05, .05, .05)	
7	(.4, .4, .05, .05, .05, .05)	
8	(.4, .05, .4, .05, .05, .05)	
9	(.4, .05, .05, .4, .05, .05)	
10	(.4, .05, .05, .05, .4, .05)	
11	(.4, .05, .05, .05, .05, .4)	
12	(.05, .4, .4, .05, .05, .05)	
13	(.05, .4, .05, .4, .05, .05)	
14	(.05, .4, .05, .05, .4, .05)	
15	(.05, .4, .05, .05, .05, .4)	
16	(.05, .05, .4, .4, .05, .05)	
17	(.05, .05, .4, .05, .4, .05)	
18	(.05, .05, .4, .05, .05, .4)	
19	(.05, .05, .05, .4, .4, .05)	
20	(.05, .05, .05, .4, .05, .4)	
21	(.05, .05, .05, .05, .4, .4)	
22	(.54, .05, .05, .12, .12, .12)	
23	(.05, .12, .12, .54, .05, .12)	
24	(.05, .12, .12, .12, .05, .54)	
25	(.12, .05, .05, .12, .54, .12)	
26	(.12, .54, .12, .05, .12, .05)	
27	(.12, .12, .54, .05, .12, .05)	$.859 \times 10^{-55}$
28	(.54, .12, .05, .12, .12, .05)	$.867 \times 10^{-55}$
29	(.54, .05, .12, .05, .12, .12)	$.905 \times 10^{-55}$
30	(.12, .12, .05, .05, .54, .12)	$.958 \times 10^{-55}$
31	(.12, .05, .12, .12, .54, .05)	$.104 \times 10^{-54}$
32	(.12, .54, .05, .12, .05, .12)	$.101 \times 10^{-54}$
33	(.12, .12, .05, .54, .12, .05)	$.983 \times 10^{-55}$
34	(.05, .05, .54, .12, .12, .12)	$.923 \times 10^{-55}$
35	(.09, .05, .05, .38, .05, .38)	$.863 \times 10^{-55}$
36	(.05, .38, .05, .09, .38, .05)	$.816 \times 10^{-55}$
37	(.05, .38, .05, .05, .09, .38)	$.786 \times 10^{-55}$
38	(.38, .09, .05, .05, .05, .38)	$.771 \times 10^{-55}$
39	(.05, .38, .38, .05, .05, .09)	$.770 \times 10^{-55}$
40	(.38, .05, .09, .38, .05, .05)	$.779 \times 10^{-55}$
41	(.09, .05, .38, .05, .05, .38)	$.788 \times 10^{-55}$

optimal. These designs are all superior to the designs in Tables 18 and 19. We note that design ξ^* in Table 11 has a large number of points of support with fairly different measures on these points of support. Therefore the general comments made about exact designs in five components still apply, and the designs in Table 20 indicate that our suggestion of obtaining sequentially optimal designs using as candidates the points of support of ξ^* is a reasonable one. It is possible, of course, to improve on the designs in Table 20 by applying Fedorov's exchange algorithm to the 111 candidates to obtain D_n-optimal designs, or by selecting as candidates the entire set of points in the design region There is no programming difficulty in applying either of these alternatives, but we have not done so because of the computing expense.

We will give only sequentially optimal designs for model II in six components. We note though, that the designs for $n = p = 27$ are D_n-optimal, and that the sequential designs are obtained by sequentially adding the candidate point of maximum variance to this D_n-optimal design.

The approximately D-optimal design ξ^* given in Table 12 contains 171 points of support. The computing expense of obtaining a 27 point D_n-optimal design for these 171 candidate points would be quite large, and we have not attempted to find such a design. Table 21 gives the sequentially optimal designs for $n = 27$ through 41 using the 81 points of support of design ξ_2 from Table 12. We note that the value of $|\underline{M}(\xi(n))|$ does not improve as n increases.

In Table 22 we give the sequentially optimal designs for $n = 27$ through 41 obtained using the 141 points of support of design ξ_1 (which is nearly D-optimal) from Table 12. Since the set of 81 points of support of ξ_2 is a subset of this set of 141 points of support, the designs in Table 22 should be at least as good as those in Table 21. In fact, these designs are the same for $n = 27$

through 34, and slightly better for $n = 35$ through 41.

We have not obtained sequentially optimal designs for this model using as candidates the 171 points of support of design ξ^*. This would require finding the 27 point D_n-optimal design from these 171 candidates, and the sequential designs for $n > 27$, and we have not obtained these designs because of the computing expense.

<u>Comments</u>. We note again that the approximately D-optimal design ξ^* for this model has many (171) points of support and widely different measures on these points (see Table 12) and therefore relatively good (in terms of $|\underline{M}(\xi(n))|$) exact designs for this model may be very difficult to obtain, and in fact, may not exist.

We have observed for model II in five components and for model I in six components that sequentially optimal designs from a large number of candidates are in general better than D_n-optimal designs from a smaller number of candidates. It would, of course, be possible to obtain better designs by not restricting the set of candidate points to be the set of points of support of a measure design. However, this would, in general, require evaluating many quadratic forms involving pxp matrices. For a large number of candidates this would not be financially feasible. Therefore, our procedure is a reasonable way of restricting the number of candidates and it has the advantage of converging to a good measure design (ξ^* if the set of candidates corresponds to the points of support of ξ^*).

6. SUMMARY AND COMMENT

We have obtained measure designs in five and six components for models with inverse terms by using a number of improvements to Fedorov's D-optimality algorithm. Among these improvements are Atwood's speed-up suggestions, our method of adding tied points of maximum variance, our method of removing measure from points of support with small variance and re-distributing this measure only among the points of support with large variance, and considerations of symmetry in reducing the region to search in finding the point of maximum variance. In obtaining various exact designs we have restricted our attention to the points of support of the measure designs, and we have used a sequential approach to obtain these designs.

We add the following comment. There are numerous criteria for selecting a response surface design; one of these is D-optimality. It follows that, while it is of interest to see what sort of designs are D- and D_n-optimal so that their basic characteristics can be noted, and made use of where possible, such designs are not necessarily "best" in any wider sense. Such a determination would demand a much wider view of the problem then we have taken here.

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Briefly reviewed are the polynomial plus inverse terms mixture models of Draper and St. John (1977a), and the approximately D-optimal (measure) and D_n-optimal (exact) designs for these models in three and four components (see Draper and St. John (1977b)). The use of Atwood's (1973) improvement to Fedorov's D-optimality algorithm is reviewed and further improvements are suggested. In addition, design region and model symmetry, and a simplified procedure for re-distributing design measure, are used to obtain measure designs in five and six components. Finally, exact designs are obtained from these measure designs.

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